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Static local field factor for spin interacting system

A Sarkar*, S Haldar[†], D Sen** and D Roy

Condensed Matter Physics Research Centre, Department of Physics,
Jadavpur University, Calcutta-700 032, India

Abstract A simple form for the static local field factor $G(q)$ which appears in the dielectric screening theory for the most general case of unpolarised interacting electron gas is proposed. A very accurate fit of Ceperley-Alder data of electron correlation energy for both spin parallel and antiparallel states in the entire density range using Levin-Wenger interpolant is obtained and used for the calculation of $G(q)$. Both the short- and long-wavelength limits of $G(q)$ are satisfied exactly in the present formulation which ensures fulfilment of number of other consistent criteria and provides some interesting results

Keywords . Electron correlation energy, local field factor, dielectric screening theory

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1. Introduction

The role of local field factor (LFF) in dielectric screening theory is very crucial [1-3]. In an earlier work [3], a good deal of attention has been paid to the static local field factor in dielectric screening function of electron gas. The test charge static dielectric function is given by

$$\varepsilon(q) = 1 - \frac{v(q)\chi_0(q)}{1+v(q)G(q)\chi_0(q)}, \tag{1}$$

where $\chi_0(q)$ is the Lindhard (noninteracting) static response function, $v(q) = 4\pi e^2 / q^2$ the Coulomb coupling factor and $G(q)$ simulates the exchange and correlation (XC) effects of the electron gas in the local approximation. This $G(q)$ is known as local field factor. A detailed discussion on $G(q)$ is provided by Sarkar *et al* [3] and also by references given therein. However, in all the existing literatures including the most recent attempts [4-7], the spin interaction of the unpolarised system is not properly treated as no distinction is made between the response of the spin-up electrons (say) to the spatial polarisation of the spin-up electrons than they do to the spatial polarisation of the spin-down electrons of the unpolarised electron gas.

* Corresponding Author
** Present address : Barasat Govt. College, Barasat 743201, West Bengal, India.
† Asansol Engineering College, Asansol-4, West Bengal, India.
E-mail : sandeep@juphys.ernet.in

2. Theory

Following Dolgov *et al* [8], one may recall that as r_s (Wigner-Seitz radius of the electrons in units of Bohr radius) is increased, the electron gas system may become unstable with respect to the formation of states with charge density wave (CDW) or spin density wave (SDW). The system becomes unstable with respect to the divergency of the corresponding response function, *i.e.* the divergency of the charge susceptibility $\chi(q)$ for CDW or the divergency of the magnetic susceptibility $\chi_m(q)$ for SDW. Following density functional theory one may calculate both the functions. In the static limit, one can define

$$\chi(q) = \frac{\chi_0(q)}{1 - v(q)[1 - G(q)]\chi_0(q)} \tag{2}$$

and

$$\chi_m(q) = \frac{-\mu_B^2 \chi_0(q)}{1 + v(q)\bar{G}(q)\chi_0(q)}. \tag{3}$$

Here $\bar{G}(q)$ is the spin function of the LFF. The functions $G(q)$ and $\bar{G}(q)$ can be written as [9]

$$G(q) = \frac{1}{2}\left[G^F(q) + G^P(q)\right] \tag{4}$$

and

$$\bar{G}(q) = \frac{1}{2}\left[G^F(q) - G^P(q)\right]. \tag{5}$$

where $G^F(q)$ and $G^P(q)$ are the LFF for electrons with parallel and antiparallel spins respectively.

The spin interaction in the theory of LFF for unpolarised electron gas, therefore, replaces $G^P(q)$ with $G(q)$. The present paper provides a brief account of $G(q)$ through a consistent evaluation of $G^F(q)$ and $G^P(q)$.

Evaluation of $G^F(q)$ requires knowledge of XC energy functional and its derivative for ferro-state of electron gas. Ceperley and Alder (CA) [10] have provided correlation energy of electron gas for ferro-state at six different r_s values from Quantum Monte Carlo (QMC) calculation. Vosko, Wilk and Nusair (VWN) [11] have fitted the QMC data for the correlation energy of CA by a Pade' type rational interpolant. The VWN fit exhibit some problem discussed in Ref. [3]. In this present paper, we have provided an improved and good fit of CA data and obtained a closed form expression for correlation energy with Levin-Weniger interpolants and the details of this fitting scheme is given in Ref. [3]. The present fit of $e_C^f(r_s)$ is made over entire density range using all the six points of QMC data of CA and U_5 interpolant is given by

$$e_C^f(r_s) = -\frac{1 + a_1 r_s + a_2 r_s^2 + a_3 r_s^3 + a_4 r_s^4}{b_0 + b_1 r_s + b_2 r_s^2 + b_3 r_s^3 + b_4 r_s^4 + b_5 r_s^5} mRyd, \quad (6)$$

where

a_1 = 0.24979381, a_2 = 0.042193510,

a_3 = 0.00273095, a_4 = 0.00003620,

b_0 = 0.011258694, b_1 = 0.00723687,

b_2 = 0.00165158, b_3 = 0.00017853,

b_4 = 7.9656334E−06 b_5 = 6.47520896E−08.

The ground state energy density of a homogenous electron gas in Local Density Approximation (LDA) may be written [12] as

$$e^{LDA}(n(r)) = e^{\text{hom}}(n(r))_{n(r)-} \quad (7)$$

The above prescription is also applicable to the spin polarised state of electron gas through their respective spin densities *via* the variable $n(r)$ defined as

$$n(r) = n_+(r) + n_-(r) \quad (8)$$

and

$$\zeta = \frac{n_+(r) - n_-(r)}{n_+(r) + n_-(r)} \quad (9)$$

where $n_\pm$ are the densities of spin polarised states.

Following VWN the exchange energy $e_X(r_s, \zeta)$ and correlation energy $e_C(r_s, \zeta)$ per particle of a homogenous electron gas for spin polarised state may be written as

$$e_X(r_s, \zeta) = e_X^P(r_s) + \left[e_X^f(r_s) - e_X^P(r_s)\right] f(\zeta)$$

$$= e_X^P(r_s) + \Delta e_X(r_s, \zeta), \quad (10)$$

$$e_C(r_s, \zeta) = e_C^P(r_s) + \left[e_C^F(r_s) - e_C^P(r_s)\right] f(\zeta)$$

$$= e_C^P(r_s) + \Delta e_C(r_s, \zeta), \quad (11)$$

where $e_X^P(r_s) = -0.916/r_s$, $e_X^F(r_s) = 2^{\frac{1}{3}} e_X^P(r_s)$, $f(\zeta) = \left[(1+\zeta)^{\frac{4}{3}} + (1-\zeta)^{\frac{4}{3}} - 2\right] / \left[2(2^{\frac{1}{3}} - 1)\right]$ and e_C^P from Ref. [3]

Now from eqs. (10) and (11), we can write

$$e_{XC}(r_s, \zeta) = e_X^P(r_s) + \Delta e_X(r_s, \zeta) + e_C^P(r_s) + \Delta e_C(r_s, \zeta).$$

From the expression of $\Delta e_C(r_s, \zeta)$, it is clear that $\Delta e_C(r_s, \zeta)$ may be expressed in a closed analytical form using eq. (6) for $e_C^F(r_s)$, eq. (2) for $e_C^P(r_s)$ of Ref. [3] and the expression for $f(\zeta)$.

Following our earlier communication [3], here we like to extract a reliable LFF $G^F(q)$ for ferromagnetic electron gas with the criteria that $G^f(q)$ must satisfy (i) exact compressibility sum rule in the low q limit (ii) positivity of pair correlation function with the fulfilment of Kimball's [9] criterion of the long wavelength limit (iii) reproduce the XC energy/particle of the homogenous electron gas (ferro-magnetic state) system under LDA. The details of the criteria and extraction of LFF for homogenous electron gas system may be found in Ref. [3]. The $G^F(q)$ function obtained in the present formulation satisfying various criteria may be given by a three parameter expression .

$$G^f(q) = A_F \qquad 1 + B_F \qquad \exp\ -C_F \qquad \}, \quad (12)$$

where k_f is the Fermi wave vector, A_F and C_F determine the two limiting behaviours of $G^F(q)$.

From first criteria we can write [3]

$$\lim_{q \to 0} G^F(q) = \gamma_0^F(r_s) \left| \frac{q}{k_f} \right.$$

where the compressibility sum rule coefficient

$$\gamma_0^F(r_s) = -\frac{k_f^2}{8\pi} \frac{d^2}{dn^2} \left(n e_{xc}^F\right)$$

$$\frac{1}{4} - \frac{\pi \alpha}{24} r_s^5 \frac{d}{dr_s} \left| r_s^{-2} \frac{d}{dr_s} e_c^F(r_s) \right|.$$

Following Kimball [9], the second criteria *i.e.* the large-q behaviour of the LFF may be obtained as follows :

$$g^P(0) = 1 - G^P(\infty) \text{ and } g^F(0) = 1 - G^F(\infty).$$

The pair correlation fucntion $g(r)$ for the unpolarised state is accordingly given by

$$g(r) = \frac{1}{2}\left[g^P(r) + g^F(r)\right].$$

Now Pauli principle asserts that $g^F(0) = 0$, which implies $G^F(\infty) = 1$ and $G^P(\infty) = 1 - 2g(0)$.

Thus without introducing serious error, we can write in first approximation:

$$Lt_{q\to\infty} \frac{1}{2}\left[G^P(q) + G^F(q)\right] = 1 - g(0),$$

and

$$Lt_{q\to\infty} \frac{1}{2}\left[G^F(q) - G^P(q)\right] = -g(0).$$

The short range correlation $g^P(0) = g^P(0, r_s)$ is taken from ladder diagramatic calculation of Yasuhara [13].

Following criterion (iii), $B^F(r_s)$ is obtained as

$$B^F(r_s) = a + br_s + cr_s^2 + dr_s \ln r_s + er_s^2 \ln r_s \,, \qquad (13)$$

where

$$a = 0.27120697 \quad b = 0.023367297 \quad c = 0.0004025675,$$

$$d = -0.0067372145 \quad e = -6.3667962E-05.$$

Finally with this, $G^F(q)$ given by eq. (12) and $G^P(q)$ from Ref. [3], $G(q)$ is evaluated and the result obtained is found to be encouraging.

3. Results and discussion

Figure 1(a) shows the variation of $e_C^F(r_s)$ (Eq. 6) with r_s over entire range of density, the result obtained is found to be in better agreement compared to the other fitted value [11] of the same. Figure 1(b) shows the variation of $\gamma_0^F(r_s)$ with r_s, for the entire density range $0 < r_s < 100$. Figure 2 shows the variation of $G^P(q)$, $G^F(q)$ and of $G(q)$ versus q at $r_s = 4$. In the case of $G(q)$, unlike $G^P(q)$, a peak structure is obtained which weakens gradually beyond the metallic density regime. The general static LFF is found to be very effective in reproducing effective pair potential in metals. In a recent *ab initio* pseudopotential study [14] the use of $G(q)$ instead of $G^P(q)$ is found to reproduce the hard-sphere description of the effective pair potential of Al, in close agreement with a very recent study [15] using embedded atom method and based on a large set of *ab initio* data, consistent with the empirical demand from the ionic pair correlation data [14].

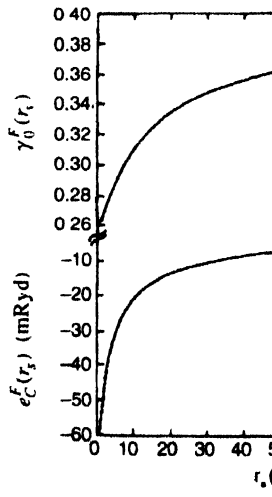

Figure 1. (a) The correlation energy / particle $e_C^F(r_s)$ in mRyd and (b) the compressibility sum rule coefficient $\gamma_0^F(r_s)$ *vs* r_s in a.u.

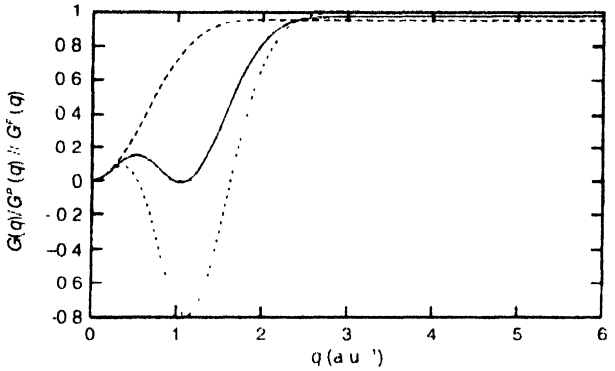

Figure 2. Variation of $G(q)$ (solid curve), $G^F(q)$ (large dashed curve) and $G^P(q)$ (small dashed curve) with q at $r_s = 4$

The obtained fit for correlation energy $e_C^F(r_s, \zeta)$ may be employed to determine the spin susceptibility of paramagnetic state. Following Vosko and Pedrew [16] in local spin density approximation (LSDA) the spin stiffness factor,

$$\alpha_{XC}(r_s) = \left(\delta^2 e_{XC}(r_s, \zeta)/\delta\zeta^2\right)_{\zeta\to 0} \qquad (14)$$

can be estimated from the long wavelength limit of the spin susceptibility enhancement. Table 1 shows the calculated spin stiffness factor from eq. (14) at various densities and compares with the results of VWN [11]. The numerical values of the spin stiffness factor given in Table 1 are the correlation only values

Table 1. Calculated values of correlational spin stiffness factor in mRyd at different r_s values

r_s in a.u.	$\alpha_C(r_s)$ present Calc	$\alpha_C(r_s)$ VWN results
0.5	147.27	100.1
1.0	106.59	79.4
2.0	72.16	60.1
3.0	57.25	49.8
4.0	48.71	43.0
5.0	42.92	38.0
6.0	38.59	34.2
7.5	33.63	28.18
10.0	27.74	23.29
15.0	20.44	17.45

i.e. the effect of exchange is not included in $\alpha_C(r_s)$. The values of $\alpha_C(r_s)$ obtained in the present calculation, are higher than corresponding VWN values. In fact, the VWN fit to $e_C(r_s)$ contains some physically undesirable singularities that cause strong differences in its derivatives.

It has been established that an interacting electron gas system shows a transition from para to ferro-state at certain value of r_s and finally at a second transition, it exhibits Wigner Crystallization [3] as the system passes to a BCC crystalline state from its usual fluid state.

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